# **FINAL REPORT FOR GRANT NAG5-11990**

TITLE:

Laboratory Studies of Thermal Energy Charge Transfer of Multiply

**Charged Ions in Astrophysical Plasmas** 

**PRINCIPAL** 

INVESTIGATOR: Victor H.S. Kwong

**INSTITUTION:** 

**Department of Physics** 

University of Nevada, Las Vegas

4505 Maryland Parkway Las Vegas, NV 89154-4002

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### A: INTRODUCTION:

The laser ablation/ion storage facility at the UNLV Physics Department has been dedicated to the study of atomic and molecular processes in low temperature plasmas. Our program focuses on the charge transfer (electron capture) of multiply charged ions and neutrals important in astrophysics. The electron transfer reactions with atoms and molecules is crucial to the ionization condition of neutral rich photoionized plasmas.

With the successful deployment of the Far Ultraviolet Spectroscopic Explorer (FUSE) and the Chandra X-ray Observatory by NASA, high resolution VUV and X-ray emission spectra from various astrophysical objects have been collected. These spectra will be analyzed to determine the source of the emission and the chemical and physical environment of the source. The proper interpretation of these spectra will require complete knowledge of all the atomic processes in these plasmas. In a neutral rich environment, charge transfer can be the dominant process. The rate coefficients need to be known accurately.

We have also extended our charge transfer measurements to KeV region with a pulsed ion beam (Wong and Kwong, 1997, Gao, Fang, and Kwong, 2001). The inclusion of this facility into our current program provides flexibility in extending the measurement to higher energies (KeV) if needed. This flexibility enables us to address issues of immediate interest to the astrophysical community as new observations are made by high resolution space based observatories.

#### B. RESEARCH SUMMARY

During the grant year, we pursue our investigation to include association reactions involving molecular ions and neutral molecules and substitution reactions between hydrogen and deuterium. Specifically, we study the following reactions:

$$H_2O^+ + D_2 \implies H_2DO^+ + D$$
 (1)

$$H_2DO^+ + H_2O \implies HDO + H_3O^+$$
 (2)

$$H_2DO^+ + D_2 -> HD_2O^+ + D + H$$
 (3)

$$HD_2O^+ + D_2 \rightarrow D_3O^+ + D + H$$
 (4)

$$CO^+ + D_2 \longrightarrow DCO^+ + D \tag{5}$$

$$CH_3^+ + D_2 \longrightarrow CH_2D^+ + D$$
 (6)

Our preliminary investigation suggests that the rate coefficients for the association reactions, i.e. (1) and (5), are of the order of 10<sup>-10</sup>cm<sup>3</sup>s<sup>-1</sup> while that for the H/D substitution reactions, i.e. (2), (3) and (4), are of the order of 10<sup>-12</sup> cm<sup>3</sup>s<sup>-1</sup> and (6) is about 10<sup>-11</sup> cm<sup>3</sup>s<sup>-1</sup>. These results may explain the hydrogen/ deuterium fractionation discrepancies in planetary atmospheres (Krasnopolsky et al., 1998, Yung and Kass 1998) and set a limit on the cosmic deuterium-

hydrogen abundance in dense interstellar cloud (Dalgarno and Lepp, 1984, Robert, Herbst, and Millar, 2002). For example, Yung et al. (1988) proposed a one-dimension photochemical model involving several physical and chemical processes that lead to the preferential escape of hydrogen over deuterium in Martian atmosphere. However, the amount of the water they estimated on Mars is too low. To reconcile the measurement (Krasnopolsky et al. 1998) with the photochemical model, Yung and Kass (1998) revise their model that the D/H ratio of the hydrogen that escapes from Mars may be determined by thermodynamic equilibrium between HD and H<sub>2</sub>O in the reaction:

$$HD + H2O \longrightarrow H2 + HDO$$
 (7)

with the partitioning of D between HD and HDO in the atmosphere defined by

$$R = (DH/H_2)/(HDO/H_2O)$$

This revised model on H/D fractionation gives a R =0.14, a value closer to measured value of 0.09. However, this will require the rate coefficient of reaction (7) to be greater then 10<sup>-23</sup>cm<sup>3</sup>s<sup>-1</sup>, 10 orders of magnitude larger than the laboratory value of 10<sup>-33</sup> cm<sup>3</sup>s<sup>-1</sup> (Lecluse & Robert, 1994). Yung and Kass (1998) suggest two possible solutions to this paradox. First, he suggests that there is an unknown reaction that can reduce the value of R in the thermodynamic equilibrium model of his. Second, there is an unknown catalyst on Mars that can raise the rate coefficient of reaction (7) by 10 orders of magnitude.

The basic assumption in Yung's model is:  $H_2O$  exists in neutral form. However, the Martian atmosphere is constantly bombarded by solar wind ions as well as x-ray, VUV, and UV from the sun. It is not unreasonable to assume that a small fraction of  $H_2O$  is in the form of  $H_2O^+$ . The presence of the  $H_2O^+$  can significantly reduce HD concentration in the Martian atmosphere by ion-molecule reactions:

$$H_2O^+ + HD \rightarrow H_2DO^+ + H$$
 (8a)

$$-> H_3O^+ + D$$
 (8b)

Our preliminary measurement on the reaction (1) i.e.  $H_2O^+ + D_2 \rightarrow H_2DO^+ + D$ , indicates a rate coefficient of the order  $10^{-10}$  cm<sup>3</sup>s<sup>-1</sup>. Even though this measurement is for  $H_2O^+$  and  $D_2$ , the  $D_2$  reaction is a good pointer to how HD will react with  $H_2O^+$ . This suggests that the rate coefficients for reaction (8a) and (8b) are of the order of  $10^{-10}$  cm<sup>3</sup>s<sup>-1</sup>, 23 orders of magnitude larger than the neutral reaction (7). Even if we were to assume that the ionization fraction of  $H_2O$  is small, the vast difference in their rate coefficients provides a significant alternate channel to remove HD from the atmosphere. This can make reaction (8a) and (8b) appear to have a significantly higher rate coefficient. Furthermore, the fast reaction (2) also suggests a rapid production of HDO thus making the R value much smaller.

We are in the process of refining these measurements. These results will form the basis for the next proposed research to NASA.

## C. PAPERS PUBLISHED AND PAPERS SUBMITTED

- "Charge transfer between C<sup>2+</sup> and H<sub>2</sub>, N<sub>2</sub>, He, and CO at eV energies", H. Gao and Victor H.S. Kwong, Accepted for publication in Physical Review A, 2003.
- "Thermal energy charge transfer between  $\underline{S^{2+}}$  and  $\underline{H_2}$ ,  $\underline{N_2}$ , and  $\underline{CO}$ ," De Chen, H. Gao, and Victor H.S. Kwong, Submitted to Physical Review A, April, 2003.
- Charge transfer of O<sup>5+</sup> and O<sup>4+</sup> with CO at kilo-electron volt energies, Gao, H. and Kwong, V.H.S., Ap.J. 567, 1272, 2002.
- Measurement of electron capture cross-sections at KeV energies and charge transfer rate coefficients at eV energies, Kwong, V.H.S., Z. Fang, H.Gao, and D. Chen, Spectroscopic Challenge of Photoionized Plasmas, ASP Conference Series, In press, 2001, Gary Ferland and Danniel Wolf Savin, eds.
- Absolute total one- and two-electron-transfer cross sections of O<sup>3+</sup> and O<sup>4+</sup>with CO at Kiloelectron-volt energies, Gao,H., Z. Fang, and V.H.S. Kwong, Phys.Rev.A63, 32704-1, 2001.
- "Measurement of Charge-Transfer-Rate Coefficients of Ground-State He<sup>+</sup> with N<sub>2</sub> and CH<sub>4</sub> at Electron-Volt Energies." Z. Fang, D. Chen and V.H.S. Kwong, Physical Review A62, 42709-1, 2000.
- "Dissaciative Charge Transfer Between Ground State He<sup>+</sup> and CO at Electron-Volt Energies," V.H.S. Kwong, D. Chen and Z. Fang, Astrophysical Journal, 536, 954, 2000.
- "Charge Transfer Between Si<sup>4+</sup> Ion and Helium at Electronvolt Energies," Z. Fang and V.H.S. Kwong, Phys. Rev. A.59, 342, 1999.

#### D. CONFERENCE PRESENTATIONS

- "Measurement of electron capture cross-sections at KeV energies and charge transfer rate coefficients at eV energies," Kwong, V.H.S., Z. Fang, H.Gao, and D. Chen, The Challenge of High Resolution X-ray to IR Spectroscopy, University of Kentucky, Lexington, Kentucky, November 15, 2000.
- "Charge transfer between S<sup>2+</sup> ions and H<sub>2</sub> at electron volt energies," Victor H.S. Kwong, De Chen, and Hui Gao, NASA Laboratory Astrophysics Workshop, Ames Research Center, Moffett Field, California, May -1 -03, 2002.

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Yung Y.L. and Kass, D.M., 1998, Science 280, 1545.

Yung Y.L., Wen, J-S., Pinto, J.P., Allen, M., Pierce, K.K., and Paulson, S., 1988, ICARUS 76, 146.